



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2021 – 10:31 AM EDT

PDB ID : 4KKI
Title : Crystal Structure of Haptocorrin in Complex with CNCbl
Authors : Furger, E.; Frei, D.C.; Schibli, R.; Fischer, E.; Prota, A.E.
Deposited on : 2013-05-06
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

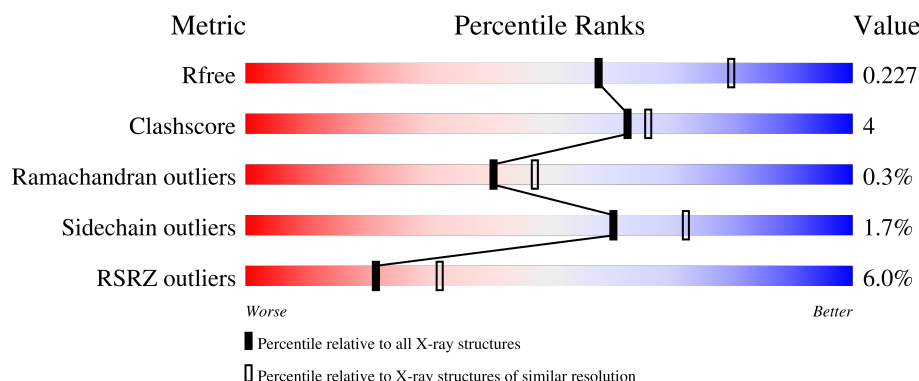
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	467	<div> <div>5%</div> <div>75%</div> <div>9%</div> <div>15%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	506	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CNC	A	508	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3519 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Transcobalamin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	398	3116	1967	515	616	18	0	0	0

There are 34 discrepancies between the modelled and reference sequences:

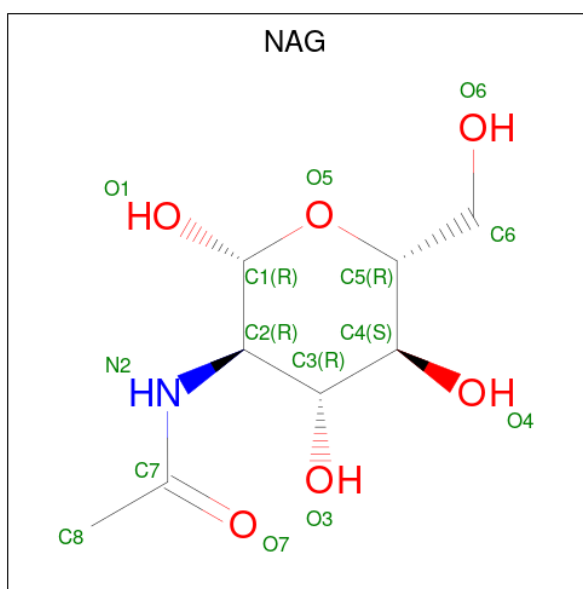
Chain	Residue	Modelled	Actual	Comment	Reference
A	411	LEU	-	expression tag	UNP P20061
A	412	VAL	-	expression tag	UNP P20061
A	413	PRO	-	expression tag	UNP P20061
A	414	ARG	-	expression tag	UNP P20061
A	415	GLY	-	expression tag	UNP P20061
A	416	SER	-	expression tag	UNP P20061
A	417	LEU	-	expression tag	UNP P20061
A	418	GLU	-	expression tag	UNP P20061
A	419	SER	-	expression tag	UNP P20061
A	420	ARG	-	expression tag	UNP P20061
A	421	GLY	-	expression tag	UNP P20061
A	422	PRO	-	expression tag	UNP P20061
A	423	PHE	-	expression tag	UNP P20061
A	424	GLU	-	expression tag	UNP P20061
A	425	GLN	-	expression tag	UNP P20061
A	426	LYS	-	expression tag	UNP P20061
A	427	LEU	-	expression tag	UNP P20061
A	428	ILE	-	expression tag	UNP P20061
A	429	SER	-	expression tag	UNP P20061
A	430	GLU	-	expression tag	UNP P20061
A	431	GLU	-	expression tag	UNP P20061
A	432	ASP	-	expression tag	UNP P20061
A	433	LEU	-	expression tag	UNP P20061
A	434	ASN	-	expression tag	UNP P20061
A	435	MET	-	expression tag	UNP P20061
A	436	HIS	-	expression tag	UNP P20061
A	437	THR	-	expression tag	UNP P20061

Continued on next page...

Continued from previous page...

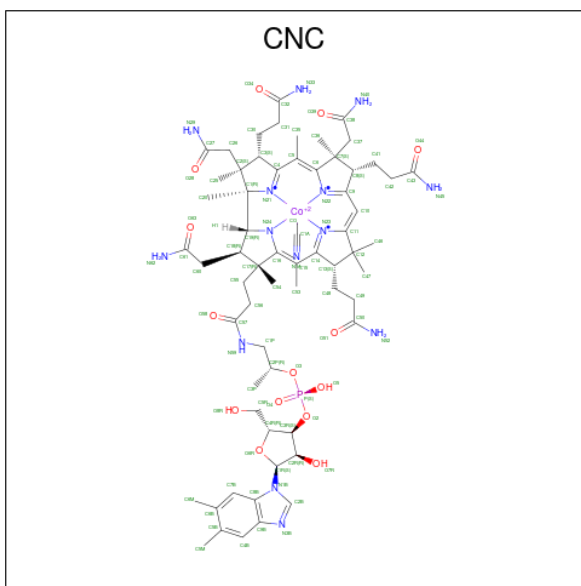
Chain	Residue	Modelled	Actual	Comment	Reference
A	438	GLY	-	expression tag	UNP P20061
A	439	HIS	-	expression tag	UNP P20061
A	440	HIS	-	expression tag	UNP P20061
A	441	HIS	-	expression tag	UNP P20061
A	442	HIS	-	expression tag	UNP P20061
A	443	HIS	-	expression tag	UNP P20061
A	444	HIS	-	expression tag	UNP P20061

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is CYANOCOBALAMIN (three-letter code: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$).

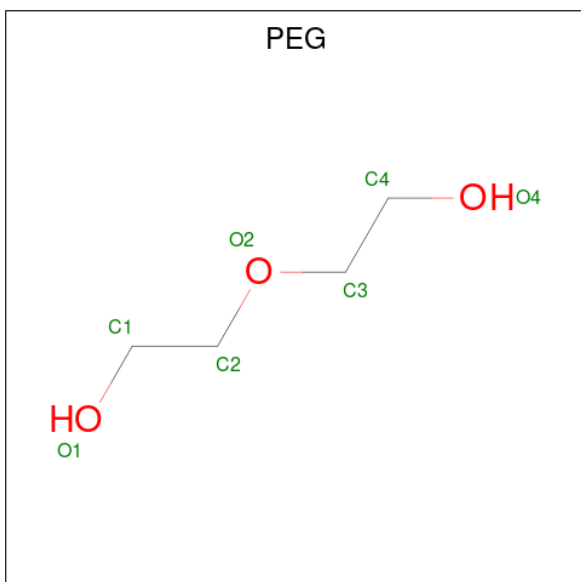


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	134	Total O 134 134	0	0

i

- Molecule 1: Transcobalamin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α , β , γ	149.89Å 149.89Å 57.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.00 – 2.35 49.06 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.00-2.35) 100.0 (49.06-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.196 , 0.226 0.197 , 0.227	Depositor DCC
R_{free} test set	1565 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3519	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, NAG, CA, CNC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/3166	0.39	0/4288

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3116	0	3061	25	0
2	A	98	0	91	1	0
3	A	93	0	87	3	0
4	A	1	0	0	0	0
5	A	77	0	110	6	0
6	A	134	0	0	2	0
All	All	3519	0	3349	29	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:HD3	5:A:515:PEG:H22	1.83	0.59
1:A:18:ASN:O	1:A:22:GLN:HG2	2.03	0.59
1:A:327:VAL:HG21	1:A:338:VAL:HG13	1.84	0.58
2:A:506:NAG:O3	2:A:506:NAG:H82	2.05	0.56
1:A:257:ALA:HA	5:A:516:PEG:H22	1.89	0.55
1:A:343:GLN:HG3	1:A:351:GLY:HA2	1.89	0.54
1:A:335:PHE:HB3	1:A:392:ALA:HA	1.89	0.54
1:A:261:PRO:HD2	5:A:517:PEG:H12	1.90	0.54
1:A:353:THR:HB	1:A:365:CYS:HB2	1.90	0.52
1:A:109:ASN:ND2	1:A:116:THR:O	2.43	0.51
1:A:139:SER:HB3	1:A:142:GLU:HB2	1.93	0.49
1:A:274:LYS:NZ	6:A:657:HOH:O	2.44	0.49
1:A:81:VAL:HA	1:A:279:ILE:HG23	1.94	0.48
1:A:17:LEU:O	1:A:21:ILE:HG12	2.15	0.46
1:A:360:GLY:HA2	5:A:517:PEG:H31	1.99	0.44
3:A:508:CNC:H252	3:A:508:CNC:C61	2.47	0.44
1:A:76:ILE:HD12	1:A:99:LEU:HD22	1.99	0.44
1:A:173:THR:HA	1:A:176:LYS:HD3	2.00	0.43
1:A:42:GLY:O	1:A:289:SER:HB3	2.18	0.43
1:A:372:ASN:HB3	1:A:375:ASP:HB2	2.00	0.43
1:A:230:VAL:HG11	1:A:277:LEU:HD12	1.99	0.43
1:A:372:ASN:HD21	5:A:518:PEG:H12	1.82	0.43
1:A:266:GLN:NE2	6:A:606:HOH:O	2.52	0.43
1:A:26:ASN:HB3	1:A:29:THR:HG22	2.01	0.43
1:A:43:ILE:HG23	1:A:292:PHE:HZ	1.85	0.42
3:A:508:CNC:H301	3:A:508:CNC:H253	1.76	0.41
3:A:508:CNC:N1A	5:A:519:PEG:H42	2.36	0.40
1:A:110:MET:HB3	1:A:110:MET:HE2	1.95	0.40
1:A:376:ARG:NH1	1:A:410:TYR:HB2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/467 (84%)	377 (96%)	16 (4%)	1 (0%)	41	47

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/414 (84%)	344 (98%)	6 (2%)	60	72

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	145	ASN
1	A	232	SER
1	A	294	ILE
1	A	311	ILE
1	A	327	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 1 is monoatomic - leaving 19 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	PEG	A	516	-	6,6,6	0.42	0	5,5,5	0.37	0
5	PEG	A	510	-	6,6,6	0.43	0	5,5,5	0.32	0
3	CNC	A	508	-	77,103,103	1.06	6 (7%)	100,171,171	1.46	20 (20%)
2	NAG	A	503	1	14,14,15	0.73	0	17,19,21	1.09	1 (5%)
5	PEG	A	512	-	6,6,6	0.43	0	5,5,5	0.32	0
5	PEG	A	517	-	6,6,6	0.43	0	5,5,5	0.36	0
5	PEG	A	520	-	6,6,6	0.43	0	5,5,5	0.26	0
5	PEG	A	514	-	6,6,6	0.46	0	5,5,5	0.19	0
2	NAG	A	504	1	14,14,15	0.53	0	17,19,21	0.65	0
2	NAG	A	505	1	14,14,15	0.53	0	17,19,21	0.69	0
2	NAG	A	501	1	14,14,15	0.56	0	17,19,21	0.74	0
2	NAG	A	507	1	14,14,15	0.49	0	17,19,21	0.85	0
2	NAG	A	506	1	14,14,15	0.42	0	17,19,21	0.81	0
2	NAG	A	502	1	14,14,15	0.67	0	17,19,21	1.24	1 (5%)
5	PEG	A	518	-	6,6,6	0.44	0	5,5,5	0.27	0
5	PEG	A	513	-	6,6,6	0.46	0	5,5,5	0.19	0
5	PEG	A	511	-	6,6,6	0.47	0	5,5,5	0.18	0
5	PEG	A	515	-	6,6,6	0.48	0	5,5,5	0.15	0
5	PEG	A	519	-	6,6,6	0.40	0	5,5,5	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	516	-	-	3/4/4/4	-
5	PEG	A	510	-	-	3/4/4/4	-
3	CNC	A	508	-	1/1/36/38	7/51/235/235	0/3/11/11
2	NAG	A	503	1	-	0/6/23/26	0/1/1/1
5	PEG	A	512	-	-	0/4/4/4	-
5	PEG	A	517	-	-	0/4/4/4	-
5	PEG	A	520	-	-	0/4/4/4	-
5	PEG	A	514	-	-	0/4/4/4	-
2	NAG	A	504	1	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1	-	3/6/23/26	0/1/1/1
2	NAG	A	501	1	-	1/6/23/26	0/1/1/1
2	NAG	A	507	1	-	2/6/23/26	0/1/1/1
2	NAG	A	506	1	-	6/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1
5	PEG	A	518	-	-	0/4/4/4	-
5	PEG	A	513	-	-	0/4/4/4	-
5	PEG	A	511	-	-	0/4/4/4	-
5	PEG	A	515	-	-	1/4/4/4	-
5	PEG	A	519	-	-	1/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	508	CNC	C20-C1	2.83	1.59	1.53
3	A	508	CNC	C17-C18	2.62	1.57	1.54
3	A	508	CNC	C11-C10	-2.36	1.36	1.40
3	A	508	CNC	C6B-C5B	2.19	1.46	1.40
3	A	508	CNC	O7R-C2R	-2.19	1.37	1.43
3	A	508	CNC	P-O5	-2.06	1.45	1.55

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	CNC	C16-C15-C14	-3.81	118.33	124.27
3	A	508	CNC	O3-C2P-C1P	3.76	114.42	106.92
3	A	508	CNC	C1-C19-N24	3.52	110.20	106.24
3	A	508	CNC	C48-C13-C12	-3.40	107.14	116.59
2	A	502	NAG	C1-O5-C5	3.40	116.80	112.19
3	A	508	CNC	O34-C32-C31	-3.39	111.12	121.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	CNC	C3R-C2R-C1R	3.34	107.29	99.89
3	A	508	CNC	C30-C3-C2	-3.27	112.20	119.13
3	A	508	CNC	C55-C17-C16	2.57	118.48	109.92
3	A	508	CNC	C47-C12-C46	-2.43	104.62	109.73
3	A	508	CNC	C36-C7-C37	-2.41	106.71	110.83
3	A	508	CNC	C31-C32-N33	2.40	123.98	116.51
3	A	508	CNC	C3-C4-C5	-2.36	123.13	131.68
3	A	508	CNC	C6-C5-C4	-2.35	120.60	124.27
3	A	508	CNC	P-O2-C3R	-2.24	111.27	119.41
3	A	508	CNC	C2-C3-C4	-2.18	99.38	101.67
3	A	508	CNC	C5B-C4B-C9B	-2.16	118.16	121.22
2	A	503	NAG	O5-C5-C4	-2.08	105.76	110.83
3	A	508	CNC	C20-C1-C19	-2.08	107.35	109.36
3	A	508	CNC	O63-C61-C60	2.08	125.24	120.87
3	A	508	CNC	C13-C14-C15	-2.05	124.23	131.68
3	A	508	CNC	C18-C60-C61	2.03	119.02	113.97

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	508	CNC	N24

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	505	NAG	C8-C7-N2-C2
2	A	505	NAG	O7-C7-N2-C2
2	A	506	NAG	C3-C2-N2-C7
2	A	506	NAG	C8-C7-N2-C2
2	A	506	NAG	O7-C7-N2-C2
3	A	508	CNC	C18-C60-C61-N62
2	A	506	NAG	O5-C5-C6-O6
2	A	506	NAG	C4-C5-C6-O6
3	A	508	CNC	C2-C3-C30-C31
2	A	507	NAG	C8-C7-N2-C2
3	A	508	CNC	C18-C60-C61-O63
2	A	505	NAG	O5-C5-C6-O6
3	A	508	CNC	C1P-C2P-O3-P
3	A	508	CNC	C3P-C2P-O3-P
2	A	507	NAG	O7-C7-N2-C2
5	A	510	PEG	O1-C1-C2-O2
5	A	519	PEG	O2-C3-C4-O4

Continued on next page...

Continued from previous page...

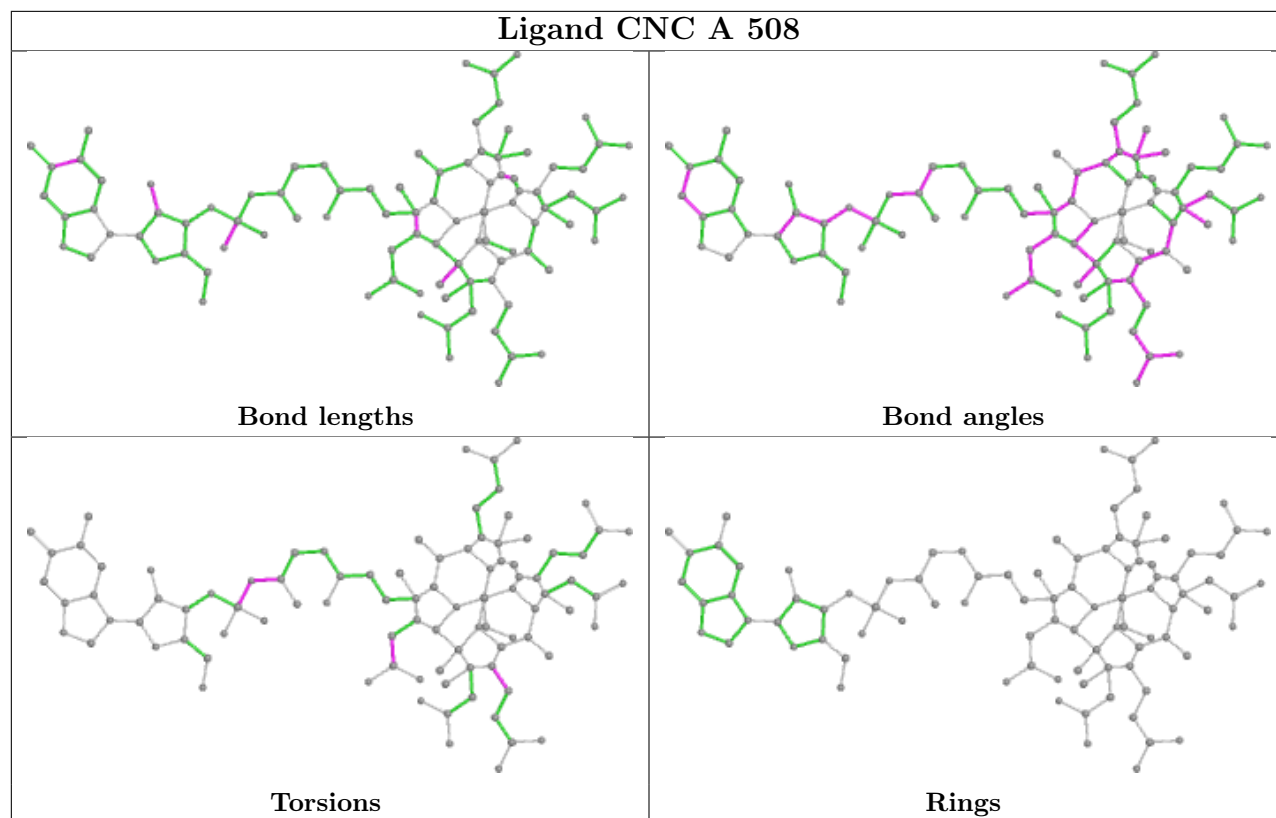
Mol	Chain	Res	Type	Atoms
3	A	508	CNC	C2P-O3-P-O2
5	A	515	PEG	O1-C1-C2-O2
5	A	510	PEG	C1-C2-O2-C3
5	A	516	PEG	O2-C3-C4-O4
5	A	516	PEG	C1-C2-O2-C3
5	A	516	PEG	O1-C1-C2-O2
5	A	510	PEG	C4-C3-O2-C2
2	A	501	NAG	C4-C5-C6-O6
2	A	506	NAG	C1-C2-N2-C7
3	A	508	CNC	C4-C3-C30-C31

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	516	PEG	1	0
3	A	508	CNC	3	0
5	A	517	PEG	2	0
2	A	506	NAG	1	0
5	A	518	PEG	1	0
5	A	515	PEG	1	0
5	A	519	PEG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	398/467 (85%)	0.32	24 (6%)	21 32	34, 54, 92, 150	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	287	SER	5.0
1	A	286	VAL	4.9
1	A	285	CYS	4.2
1	A	308	GLN	3.9
1	A	182	GLY	3.3
1	A	344	LYS	3.3
1	A	330	LEU	3.2
1	A	288	ALA	3.2
1	A	310	TYR	3.0
1	A	329	VAL	2.8
1	A	284	SER	2.7
1	A	283	SER	2.6
1	A	341	LYS	2.5
1	A	314	ASN	2.5
1	A	398	ARG	2.4
1	A	184	ILE	2.3
1	A	232	SER	2.3
1	A	325	THR	2.2
1	A	312	SER	2.2
1	A	324	PHE	2.2
1	A	332	GLY	2.2
1	A	315	TYR	2.1
1	A	399	ASN	2.0
1	A	410	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

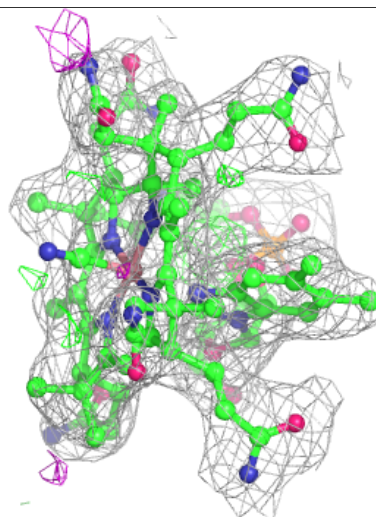
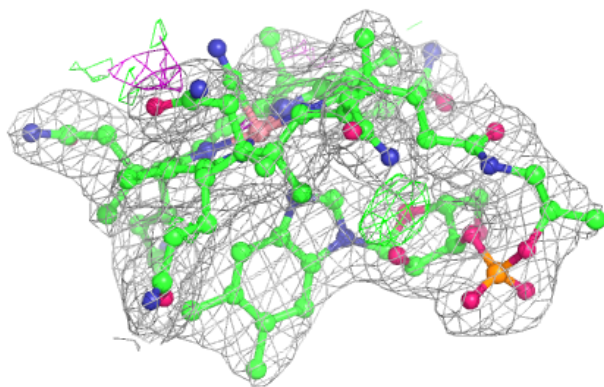
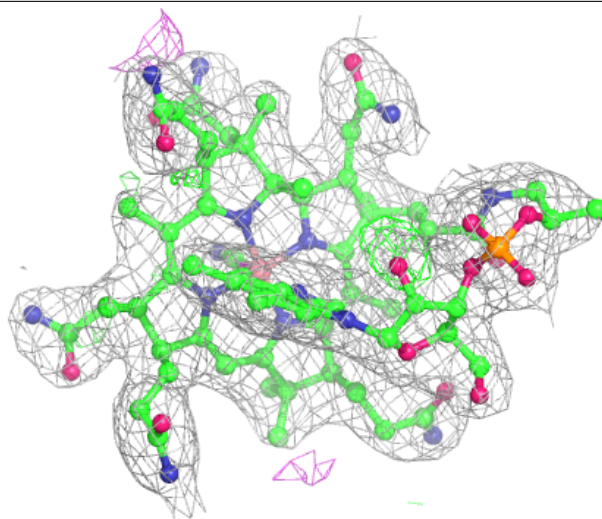
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PEG	A	515	7/7	0.61	0.20	59,65,68,79	0
2	NAG	A	505	14/15	0.64	0.36	105,129,139,146	0
5	PEG	A	513	7/7	0.68	0.24	79,84,90,92	0
5	PEG	A	520	7/7	0.69	0.34	61,84,90,95	0
2	NAG	A	506	14/15	0.74	0.45	111,125,131,131	0
5	PEG	A	519	7/7	0.75	0.21	55,65,79,81	0
5	PEG	A	510	7/7	0.76	0.37	55,61,71,79	0
5	PEG	A	516	7/7	0.79	0.20	73,89,94,98	0
5	PEG	A	518	7/7	0.80	0.14	83,93,96,97	0
5	PEG	A	517	7/7	0.81	0.21	76,77,84,85	0
5	PEG	A	511	7/7	0.81	0.27	68,74,78,81	0
5	PEG	A	512	7/7	0.83	0.29	76,79,81,87	0
2	NAG	A	507	14/15	0.83	0.34	105,114,121,125	0
5	PEG	A	514	7/7	0.84	0.24	53,60,71,74	0
2	NAG	A	501	14/15	0.87	0.20	67,79,90,97	0
2	NAG	A	502	14/15	0.87	0.22	76,86,91,91	0
2	NAG	A	503	14/15	0.92	0.18	63,70,80,82	0
4	CA	A	509	1/1	0.94	0.17	101,101,101,101	0
2	NAG	A	504	14/15	0.94	0.20	63,78,88,92	0
3	CNC	A	508	93/93	0.98	0.15	23,42,60,72	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CNC A 508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.